DESCRIPTION

Written for drug developers rather than computer scientists, this monograph adopts a systematic approach to mining scientific data sources, covering all key steps in rational drug discovery, from compound screening to lead compound selection and personalized medicine. Clearly divided into four sections, the first part discusses the different data sources available, both commercial and non-commercial, while the next section looks at the role and value of data mining in drug discovery. The third part compares the most common applications and strategies for polypharmacology, where data mining can substantially enhance the research effort. The final section of the book is devoted to systems biology approaches for compound testing.

Throughout the book, industrial and academic drug discovery strategies are addressed, with contributors coming from both areas, enabling an informed decision on when and which data mining tools to use for one's own drug discovery project.

ABOUT THE AUTHOR

Currently VP of Business Development at Prestwick Chemical SAS, Rémy Hoffmann studied pharmacy at the University Louis Pasteur in Strasbourg, France, and gained his doctorate in medicinal chemistry. After 17 years spent at what is now Accelrys, where he worked on pharmacophore perception methods, he joined Thomson Reuters as a regional sales manager. Here he learnt the importance of curated scientific data, and the need to develop methods for mining this data so as to extract accurate information to support the decisionmaking process, and thus arrive at the knowledge stage. In his current role, Dr. Hoffmann
oversees the deployment of Prestwick Chemical’s products and services to the drug discovery community, both in the pharma and biotech industries, as well as within the academic scientific community.

Arnaud Gohier studied organic chemistry at the University of Le Mans and Nantes (France). He received his PhD in Molecular Modeling from the University of Joseph Fourier in Grenoble (France). In 1999, he joined the French pharmaceutical company Servier. Dr Gohier’s main areas of interest are drug design and chemoinformatics.

Pavel Pospisil has been Manager of Computational Chemistry at Philip Morris International, R&D in Neuchatel, Switzerland, since 2008. He holds a BSc in biochemistry from the University of Joseph Fourier in Grenoble, France, and an MSc in biochemical engineering from the Institute of Chemical Technology in Prague, Czech Republic, and received his PhD in natural sciences from the Swiss Federal Institute of Technology (ETH), Zurich. He carried out his postdoctoral studies at ETH Zurich and with the pharmaceutical company, Arpida, now Evolva. In 2004, Dr. Pospisil became a postdoctoral fellow and research associate at Harvard Medical School, Boston, USA, where he focused on data mining for cancer targets and the discovery of low molecular radiolabeled cancer imaging analogs. In 2008, he took up a position as consultant at Hoffmann-La-Roche, Basel, Switzerland. His current interests are the automatic processing of molecules and computational toxicology.

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